

Quantum Mechanics

- 1) It deals with the atomic particle and sub-atomic particle.

- 2) Newton's law is not directly used.

- 3) It is the most general form of physics.

Classical Mechanics

- 1) It deals with the bulky particle.

- 2) Newton's law and its formulation is used.

- 3) It is the special case of the quantum mechanics.

* Inadequacy of Classical Mechanics:

- 1) Stability of an atom can't be explained.

- 2) The discrete energy structure of an electron of an atom can't be explained.

- 3) It can't explain the spectrum of black body radiation.

- 4) It can't explain photoelectric effect, Compton effect, etc.

- 5) It can't explain the variation in specific heat capacity of solid with temperature.

* De Broglie Principle

It states that each particle in motion has its wave nature and the wave length is obtained by

$$\lambda = \frac{h}{p}$$

$$\lambda = \frac{h}{mv}$$

where, h = Planck's constant.

λ = wavelength

$p = \text{momentum}$.

Proof:

According to Planck's black body radiation, the energy is written by

$$E = h\nu \quad (1)$$

Again, from Einstein's theory of relativity,

$$E = mc^2 \quad (11)$$

From eqⁿ (1) & (11), we get

$$h\nu = mc^2$$

$$h \frac{c}{\lambda} = mc^2$$

$$\lambda = \frac{h}{mc}$$

This is true for the particle having velocity c , i.e., speed of light.

In general form, the above formula is written as

$$\lambda = \frac{h}{mv}$$

* Concept of De-Broglie principle:

- 1) Nature loves symmetry.
- 2) Parallelism between motion of particle in mechanics and the motion of light in optics.
- 3) Involvement of integer in physics

→ If the moving particle has K.E. (E) then,

$$E = \frac{1}{2}mv^2$$

$$= \frac{1}{2} \frac{(mv)^2}{m}$$

$$= \frac{1}{2} \frac{p^2}{m}$$

$$\text{or, } p^2 = 2mE$$

$$\text{or, } p = \sqrt{2mE}$$

$$\text{Then, } \lambda = \frac{h}{\sqrt{2mE}} \quad \text{--- (i)}$$

→ If the energy of the particle is due to thermal energy

$$E = \frac{3}{2} K_B T \quad \text{--- (ii)}$$

where, $K_B \rightarrow$ Boltzmann constant

$T =$ temp in Kelvin

Using eqⁿ (ii) in (i), we get.

$$\lambda = \frac{h}{\sqrt{2m \cdot \frac{3}{2} K_B T}}$$

$$\text{or, } \lambda = \frac{h}{\sqrt{3m K_B T}} \quad \text{--- (iii)}$$

→ If the energy of the particle is given by applied potential difference,

$$E = qV - (iv)$$

Then,

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$\lambda = \frac{h}{\sqrt{2mqV}} - (v)$$

The wave length given by above formula (i), (iii) and (v) is applicable for non-relativistic case ($v \ll c$)

If the $v \approx c$ i.e. the relativistic case the wave length of particle is given as.

$$E = \sqrt{p^2 c^2 + m_0^2 c^4} ; \text{ the energy of particle.}$$

where,

$p \rightarrow$ momentum

$c \rightarrow$ speed of light.

$m_0 \rightarrow$ rest mass.

Again,

$$E = m_0 c^2 + E_k.$$

From above formula,

$$\sqrt{p^2 c^2 + m_0^2 c^4} = m_0 c^2 + E_k.$$

Squaring, we get

$$p^2 c^2 + m_0^2 c^4 = m_0^2 c^4 + 2 m_0 c^2 E_k + E_k^2$$

$$\text{or, } p^2 c^2 = E_k (E_k + 2m_0 c^2).$$

$$\therefore p = \frac{\sqrt{E_k (E_k + 2m_0 c^2)}}{c}$$

$$\therefore \lambda = \frac{h}{p} = \frac{h}{\frac{\sqrt{E_k (E_k + 2m_0 c^2)}}{c}}$$

$$\lambda = \frac{hc}{\sqrt{(E_k + 2m_0 c^2) E_k}}$$

$$\lambda = \frac{hc}{\sqrt{(E_k)^2 + E_k \cdot 2m_0 c^2}}$$

$$\text{or, } \lambda = \frac{hc}{\sqrt{E_k \cdot 2m_0 c^2 \left(\frac{E_k}{2m_0 c^2} + 1 \right)}}$$

$$\lambda = \frac{hc}{\sqrt{E_k^2 (1 + \frac{2m_0 c^2}{E_k})}}$$

$$\text{or, } \lambda = \frac{h}{\sqrt{2m_0 E_k \left(1 + \frac{E_k}{2m_0 c^2} \right)}}$$

If $E_k \ll \underbrace{2m_0 c^2}_{\text{rest mass energy}}.$

$$\lambda = \frac{h}{\sqrt{2m_0 E_k}}$$

Numericals.

i) calculate the wave length of the thermal neutron at

27°C.

mass of neutron = 1.67×10^{-27} kg.

Planck's constant = 6.67×10^{-34} J s.

Boltzmann constant = 1.376×10^{-23} J K⁻¹.

→ Solⁿ:

Temperature (T) = (27 + 273) K = 300 K.

$$\text{wavelength } \lambda = \frac{h}{\sqrt{3mk_B T}}$$

$$= \frac{6.67 \times 10^{-34}}{\sqrt{3 \times 1.67 \times 10^{-27} \times 1.376 \times 10^{-23} \times 300}}$$

$$= 1.475 \times 10^{-10} \text{ m}$$

$$= 1.475 \text{ Å}.$$

3). Find the energy of the neutron in the unit of eV whose wavelength is given by 1 Å.

→ Solⁿ:

$$\text{Energy} = \text{eV}$$

$$\frac{hc}{\lambda} = \text{eV}.$$

$$\text{Energy} = h\nu = \frac{hc}{\lambda}$$

$$= \frac{6.67 \times 10^{-34} \times 3 \times 10^8}{10^{-10}}$$

$$= 2.001 \times 10^{-15} \text{ J}.$$

$$= 3.2 \times 10^{-29} \text{ eV}.$$

4) what voltage must be applied to an electron microscope to produce electron of 0.5 Å.

→ Solⁿ:

to neutron we know,

$$h\nu = eV$$

$$\frac{hc}{\lambda} = eV$$

$$\nu = \frac{hc}{e\lambda} = \frac{6.67 \times 10^{-34} \times 3 \times 10^8}{1.6 \times 10^{-19} \times 0.5 \times 10^{-10}} = 25012.5 \text{ Volt.}$$

- 5) Calculate the de-Broglie wavelength of an α -particle accelerated through a p.d. of 2000 V. Mass of proton $= 1.67 \times 10^{-27} \text{ kg}$.

$$E = eV = 1.6 \times 10^{-19} \times 2000 = 3.2 \times 10^{-16} \text{ eV} \times 2.$$

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$= \frac{6.67 \times 10^{-34}}{\sqrt{2 \times 1.67 \times 10^{-27} \times 3.2 \times 10^{-16} \times 2}}$$

$$= \frac{4.56 \times 10^{-13} \text{ m}}{\sqrt{2}} = 3.22 \times 10^{-13} \text{ m}.$$

- 6) Find the wavelength of wave associated with an electron moving energy 1 MeV.
→ Soln:-

$$h\nu = eV$$

$$\frac{hc}{\lambda} = eV$$

$$\lambda = \frac{hc}{eV} = \frac{6.67 \times 10^{-34} \times 3 \times 10^8}{10^6 \times 1.6 \times 10^{-19}}$$

$$\therefore \lambda = 2.001 \times 10^{-31} \text{ m} \cdot 1.25 \times 10^{-12} \text{ m}.$$

2) Calculate the energy of proton having de-broglie wavelength 0.5 fm .

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$0.5 \times 10^{-15} = \frac{6.64 \times 10^{-34}}{\sqrt{2 \times 1.67 \times 10^{-27} \times E}}$$

$$2 \times 1.67 \times 10^{-27} \times E = 1.7798 \times 10^{-36}$$

$$\therefore E = 5.328 \times 10^{-10} \text{ eV}.$$

2) Calculate the de-broglie wavelength of an electron in the 1st orbit (Bohr's) of H-atom.

$$\lambda = \frac{h}{p}$$

Also,

$$p = \frac{nh}{2\pi r}$$

$$\text{So, } \lambda = \frac{h}{p}$$

$$= \frac{nh}{2\pi}$$

$$= \frac{2\pi}{n}$$

$$\text{For } n=1, \lambda = 2\pi$$

$$\therefore \lambda = 2\pi \text{ m}.$$

Energy in first Bohr's orbit of hydrogen atom

$$= -\frac{(13.6)}{1^2} \text{ eV}$$

$$= -13.6 \times 1.6 \times 10^{-19} \text{ J}$$

From de-Broglie wave length,

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$= \frac{6.6 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 13.6 \times 1.6 \times 10^{-19}}}$$

$$= 3.31 \times 10^{-10} \text{ m}$$

Heisenberg's uncertainty principle:

→ Canonical conjugate physical quantity can't be simultaneously measured:

$$\Delta E \times \Delta t \approx \hbar$$

$$\Delta L \times \Delta \theta \approx \hbar$$

$$\Delta x \times \Delta p \approx \hbar$$

It states that it is not possible to measure two canonical conjugate physical quantity accurately simultaneously, if we measure one accurately, then there occur on the another and vice versa. The product of their errors are given by:

$$\Delta x \times \Delta p \approx \hbar$$

where,

$$\text{where, } \hbar = \frac{h}{2\pi}$$

$\Delta x \rightarrow$ error in position

$\Delta p \rightarrow$ error in momentum.

similarly,

$$\Delta E \times \Delta t \approx \hbar$$

$\Delta E \rightarrow$ error in energy

$\Delta t \rightarrow$ error in time.

and,

$$\Delta L \times \Delta \theta \approx \hbar$$

$\Delta L \rightarrow$ error in angular momentum.

$\Delta \theta \rightarrow$ error in angle of rotation.

Sneetha
Potharex.

1. Calculate the uncertainty in the measurement of velocity of an electron in hydrogen atom of radius $1\text{\AA}$.

→ Here, $\Delta x = 1\text{\AA} = 10^{-10}\text{m}$

$$h = 6.62 \times 10^{-34} \text{Js}$$

$$\text{Then } \hbar = \frac{h}{2\pi} = \frac{6.62 \times 10^{-34}}{2\pi} = 1.05 \times 10^{-34} \text{Js}$$

$$\Delta p = ?$$

$$\text{We know, } \Delta x \cdot \Delta p = \hbar$$

$$\therefore \Delta p = \frac{\hbar}{\Delta x} = \frac{1.05 \times 10^{-34}}{10^{-10}} = 1.05 \times 10^{-24}$$

$$\text{mass of electron } (m_e) = 9.04 \times 10^{-31} \text{kg}$$

$$\Delta v = ?$$

$$\text{We know, } \Delta p = m \cdot \Delta v$$

$$\therefore \Delta v = \frac{\Delta p}{m} = \frac{1.05 \times 10^{-24}}{9.04 \times 10^{-31}} = 1.16 \times 10^6 \text{m/s}$$

$\therefore$ The uncertainty in measurement of velocity of an electron in hydrogen atom of radius $1\text{\AA}$ is $1.16 \times 10^6 \text{m/s}$

2. The average period that elapses between the excitation of an electron and the time of emission of radiation is 10^{-8}sec . Find the uncertainty in the energy emitted and uncertainty in the frequency of light emitted.

→ Here, $\Delta t = 10^{-8} \text{s}$

$$h = 6.62 \times 10^{-34} \text{Js}$$

$$\text{Then } \hbar = \frac{h}{2\pi} = \frac{6.62 \times 10^{-34}}{2\pi} = 1.05 \times 10^{-34} \text{Js}$$

$$\Delta E = ?$$

$$\text{We have, } \Delta E \cdot \Delta t = \hbar$$

$$\therefore \Delta E = \frac{\hbar}{\Delta t} = \frac{1.05 \times 10^{-34}}{10^{-8}} = 1.05 \times 10^{-26} \text{J}$$

$\therefore$ Uncertainty in energy emitted = $1.05 \times 10^{-26} \text{J}$

Now, $\Delta f = ?$

We have, $\Delta E = h \Delta f$

$$\therefore \Delta f = \frac{\Delta E}{h} = \frac{1.05 \times 10^{-26}}{6.62 \times 10^{-34}} = 1.5 \times 10^7 \text{ Hz}$$

$\therefore$ The uncertainty in frequency of light emitted is $1.5 \times 10^7 \text{ Hz}$

3) Find the smallest possible uncertainty in the position of an electron moving with a velocity $3 \times 10^7 \text{ m/s}$.

$\rightarrow$ Here, $\Delta v = 3 \times 10^7 \text{ m/s}$

$$\Delta = 10^{-15} \text{ m}$$

$$m_e = 9.04 \times 10^{-31} \text{ kg}$$

$$h = 6.62 \times 10^{-34} \text{ Js}$$

$$\hbar = \frac{h}{2\pi} = \frac{6.62 \times 10^{-34}}{2\pi} = 1.05 \times 10^{-34} \text{ Js}$$

$$\text{Then, } \Delta p = m \Delta v$$

$$= 9.04 \times 10^{-31} \times 3 \times 10^7$$

$$= 2.7 \times 10^{-23}$$

$$\text{Now, } \Delta x \cdot \Delta p = \hbar$$

$$\therefore \Delta x = \frac{\hbar}{\Delta p} = \frac{1.05 \times 10^{-34}}{2.7 \times 10^{-23}} = 3.8 \times 10^{-12} \text{ m}$$

$\therefore$ Uncertainty in position of electron = $3.8 \times 10^{-12} \text{ m}$

4) Assuming that an electron is inside nucleus of radius 10^{-15} m . Using uncertainty relation, estimate the kinetic energy of electron in eV.

$\rightarrow$ Here, $\Delta x = 10^{-15} \text{ m} \times 2$ (along the ~~radi~~ diameter)

$$\hbar = 1.05 \times 10^{-34} \text{ Js}$$

$$\text{Then, } \Delta x \cdot \Delta p = \hbar$$

$$\Delta p = \frac{\hbar}{\Delta x} = \frac{1.05 \times 10^{-34}}{10^{-15}} = 1.05 \times 10^{-19}$$

$$m_e = 9.04 \times 10^{-31} \text{ kg}$$

$$\text{we know, } \Delta p = m_e \Delta v$$

$$\begin{aligned} \Delta v &= \Delta p = \frac{1.05 \times 10^{-19}}{9.04 \times 10^{-31}} = 1.16 \times 10^{11} \text{ m/s} \\ \text{Now, } \Sigma &= \frac{1}{2} m (\Delta v)^2 \\ &= \frac{1}{2} \times 9.04 \times 10^{-31} \left(\frac{1.16 \times 10^{11}}{2} \right)^2 \\ &= 6.09 \times 10^{-9} \text{ J} / 4 \\ &= 6.09 \times 10^{-9} \text{ eV} \\ &= \frac{1.6 \times 10^{-19} \times 4}{3.8 \times 10^{-20} \text{ eV} / 4} = 0.95 \times 10^{10} \text{ eV} \end{aligned}$$

practically not possible because $\Delta v > 3 \times 10^8 \text{ m/s}$.

5) The hydrogen atom is nearly 10^{-8} cm in size. Calculate the uncertainty applying the uncertainty relation in velocity of the electron.

$$\rightarrow \text{Here, } \Delta x = 10^{-8} \text{ cm} = 10^{-10} \text{ m}$$

$$\hbar = 1.05 \times 10^{-34} \text{ Js}$$

$$\text{then, } \Delta x \cdot \Delta p = \hbar$$

$$\therefore \Delta p = \frac{\hbar}{\Delta x} = \frac{1.05 \times 10^{-34}}{10^{-10}} = 1.05 \times 10^{-24}$$

Then,

$$\Delta p = m \Delta v$$

$$\therefore \Delta v = \frac{\Delta p}{m}$$

$$= \frac{1.05 \times 10^{-24}}{9.04 \times 10^{-31}}$$

$$= 1.16 \times 10^6 \text{ m/s}$$

6) The speed of a bullet (50 g) and a speed of the electron ($9.1 \times 10^{-31} \text{ kg}$) are measured to be same (300 m/s) with an uncertainty of 0.01%. with what fundamental accuracy could we have the position if the position is measured simultaneously with the speed in the same experiment.

→ Here, $v = 300 \text{ m/s}$
 then, $\Delta v = 300 \times 0.01\%$
 $= 3 \times 10^{-2} \text{ m/s}$

$$m_e = 9.1 \times 10^{-31} \text{ kg}$$

$$\therefore \Delta p = m_e \times \Delta v$$

$$= 9.1 \times 10^{-31} \times 3 \times 10^{-2}$$

$$= 2.7 \times 10^{-32}$$

Now,

$$\Delta p \cdot \Delta x = \hbar$$

$$\therefore \Delta x = \frac{\hbar}{\Delta p} = \frac{1.05 \times 10^{-34}}{2.7 \times 10^{-32}} = 3.8 \times 10^{-3} \text{ m}$$

$\therefore$ Uncertainty in position of electron $= 3.8 \times 10^{-3} \text{ m}$

Now,

$$\text{mass of bullet } (m_b) = 500 \text{ gm} = 0.5 \text{ kg}$$

$$\therefore \Delta p = m_b \times \Delta v$$

$$= 0.5 \times 3 \times 10^{-2}$$

$$= 0.015$$

$$\text{Now, } \Delta p \cdot \Delta x = \hbar$$

$$\therefore \Delta x = \frac{\hbar}{\Delta p} = \frac{1.05 \times 10^{-34}}{0.015} = 7 \times 10^{-33} \text{ m}$$

$\therefore$ Uncertainty in position of bullet $= 7 \times 10^{-33} \text{ m}$

3)

$$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$$

$$= \frac{9.04 \times 10^{-31}}{\sqrt{1 - \frac{(3 \times 10^8)^2}{(3 \times 10^8)^2}}}$$

$$= \frac{9.04 \times 10^{-31}}{\sqrt{1 - 1}}$$

$$m = 9.0855 \times 10^{-31} \text{ m/s}$$

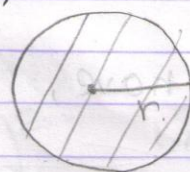
↑ use this m.

★ Application of Heisenberg's uncertainty principle.

1) Electron does not exist inside the nucleus.

⇒ Let us assume that an electron exists inside the nucleus as shown in figure. Then, the maximum possible error in the measurement of its position is

$$\Delta x = 2r = 2 \times 10^{-14} \text{ m}$$



$$\Rightarrow \Delta x = 2r = 2 \times 10^{-14} \text{ m}$$

Then,

using uncertainty relation, Fig: Nucleus

$$\Delta x \Delta p \approx h$$

$$\Delta p = \frac{h}{2\pi \Delta x} = \frac{1.05 \times 10^{-34}}{2 \times 10^{-14}}$$

$$= 5.25 \times 10^{-21} \text{ kg m/s}$$

The error in velocity Δv be obtained as.

$$\Delta p = m \Delta v$$

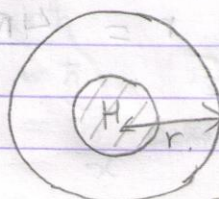
$$\text{or } \Delta v = \frac{\Delta p}{m} = \frac{5.25 \times 10^{-21}}{9.1 \times 10^{-31}}$$

$$= 5.76 \times 10^9 \text{ m/s}$$

which is greater than speed of light

⇒ Electron does not exist inside the nucleus.

2) It is used to determine the Bohr's radius of H-atom and the total energy of the electron in Bohr's orbit.



$$PE = K \frac{Qq}{r} = K \frac{(e)(e)}{r} = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{r}$$

Fig: H atom.

→ The total energy of the electron in the H-atom is

$$E = KE + PE$$

$$\text{or, } E = \frac{p^2}{2m} + \left(-\frac{e^2}{4\pi\epsilon_0 r} \right)$$

$$\text{or, } E = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} \quad \text{--- (1)}$$

we have,

$$\Delta x \Delta p \approx h$$

$$x \Delta p \approx h$$

$$\text{or, } p = \frac{h}{x} = \frac{h}{r} \quad \text{--- (2)}$$

using eqⁿ (2) in (1), we get.

$$E = \frac{h^2}{2mr^2} - \frac{e^2}{4\pi\epsilon_0 r} \quad \text{--- (3)}$$

This energy has the minimum value.

$$\text{so, } \frac{dE}{dr} = -\frac{2h^2}{2mr^3} + \frac{e^2}{4\pi\epsilon_0 r^2}$$

For minimum,

$$\frac{dE}{dr} = 0$$

$$\text{or, } -\frac{h^2}{mr^3} + \frac{e^2}{4\pi\epsilon_0 r^2} = 0$$

$$\text{or, } \frac{h^2}{mr^3} = \frac{e^2}{4\pi\epsilon_0 r^2}$$

$$\text{or, } r = \frac{4\pi\epsilon_0 h^2}{me^2} = \frac{4\pi\epsilon_0 \times h^2}{me^2}$$

$$\text{or, } \boxed{r = \frac{E_0 h^2}{\pi m e^2}} \quad \text{--- (4)}$$

which is the required value for Bohr's radius.

Using eqⁿ (4) in (3), we get,

$$\begin{aligned} E &= \frac{h^2}{2m} \left(\frac{E_0 h^2}{\pi m e^2} \right)^2 - \frac{e^2}{4\pi E_0 \left(\frac{E_0 h^2}{\pi m e^2} \right)} \\ &= \frac{h^2 / 4\pi^2}{2m \cdot \frac{E_0^2 h^4}{\pi^2 m^2 e^4}} - \frac{m e^4}{4 E_0^2 h^2} \\ &= \frac{m e^4}{8 E_0^2 h^2} - \frac{m e^4}{4 E_0^2 h^2} \end{aligned}$$

$$\text{or, } \boxed{E = -\frac{m e^4}{8 E_0^2 h^2}}$$

which is reqd. expression for energy in Bohr's orbit.

3) It is used to determine minimum energy in harmonic oscillator.

⇒ Here, $E = KE + PE$

$$\text{Total energy} = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$$

$$E = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 \quad \text{--- (1)}$$

$$\text{or } \Delta p = h$$

we have,

$$\Delta x \Delta p \approx h$$

$$x \Delta p \approx h$$

$$\text{or, } p = \frac{h}{x} \quad \text{--- (2)}$$

using (2) in (1) we get,

$$E = \frac{(\hbar/x)^2}{2m} + \frac{1}{2} m \omega^2 x^2$$
$$= \frac{\hbar^2}{2m x^2} + \frac{1}{2} m \omega^2 x^2 \quad \text{--- (3)}$$

This energy has minimum value

$$\frac{dE}{dx} = (-2) \frac{\hbar^2}{2m x^3} + 2 \times \frac{1}{2} m \omega^2 x$$

$$\frac{dE}{dx} = -\frac{\hbar^2}{m x^3} + m \omega^2 x \quad \text{--- (4)}$$

For min^m,

$$\frac{dE}{dx} = 0$$

$$-\frac{\hbar^2}{m x^3} + m \omega^2 x = 0$$

$$m \omega^2 x = \frac{\hbar^2}{m x^3}$$

$$\text{or, } x^4 = \frac{\hbar^2}{m^2 \omega^2}$$

$$\text{or, } x^2 = \frac{\hbar}{m \omega}$$

$$\therefore x = \sqrt{\frac{\hbar}{m \omega}} \quad \text{--- (5)}$$

which is the required value for x .

using eqⁿ (5) in (3)

$$E = \frac{1}{2} \hbar \omega + \frac{1}{2} m \omega^2 \frac{\hbar}{m \omega}$$

$$E = \frac{\hbar \omega}{2} + \frac{\hbar \omega}{2}$$

$$E = \hbar \omega$$

$$\boxed{E = \hbar \omega}$$

The actual value for minimum energy in Harmonic oscillator is $\frac{1}{2} \hbar \omega$.

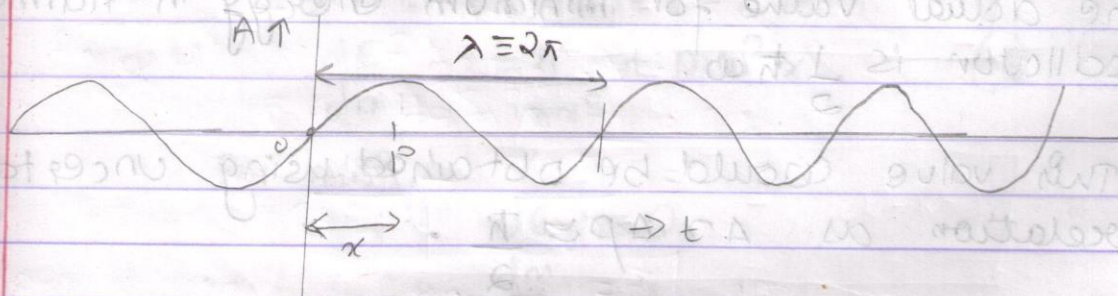
This value could be obtained using uncertainty relation as $\Delta x \Delta p \approx \frac{\hbar}{2}$.

* Wave / wave equation / wave function:

Wave : It is the form of disturbance which transfer energy from one place to another place.



Wave equation:



$$y = A \sin \omega t$$
$$y = A \sin (\omega t - \phi)$$

Consider a wave travelling from left to right in a medium as shown in fig. The particle at point O is disturbed by the wave earlier than the particle at point P, i.e., there is phase difference in vibration of the particle at pt O and P respectively. The eqⁿ of motion of the particle at O is $y = a \sin \omega t$ and the eqⁿ of the particle at point P is given as

$$y = A \sin (\omega t - \phi) \quad \text{--- (1)}$$

where ϕ is phase difference.

Again, we have

For the path diff λ phase diff is 2π

$$\frac{2\pi}{\lambda} x = \phi \quad (\text{let})$$

Then,

$$y = A \sin \left(\omega t - \frac{2\pi}{\lambda} x \right)$$

$$y = A \sin (\omega t - kx)$$

where, $k = \frac{2\pi}{\lambda}$ is wave vector or propagation constant.

$$y = A \sin \left(\frac{2\pi}{T} t - \frac{2\pi}{\lambda} x \right)$$

$$\text{or, } y = A \sin 2\pi \left(\frac{t}{T} - \frac{x}{\lambda} \right)$$

The particle velocity is different from wave velocity.
The particle velocity is obtained by $v = \frac{dy}{dt}$

$$= A\omega \cos(\omega t - kx)$$

And the wave velocity is obtained by.

$$v = f\lambda$$

This is also called phase velocity because phase diff is moving with same velocity as that of wave.

$$\psi = (2\pi f) \left(\frac{\lambda}{2\pi} \right) = (2\pi f) \cdot \left(\frac{2\pi}{\lambda} \right)$$

$$\boxed{\psi = \frac{\omega}{k}}$$

Again,

$$\boxed{y = A \sin(\omega t - kx)}$$

In exponential form.

$$\boxed{y = A e^{-i(\omega t - kx)}}$$

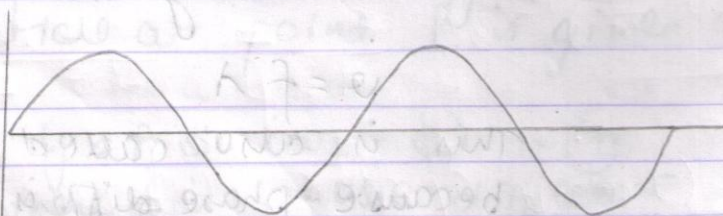
In more general form.

$$\boxed{\psi(r, t) = A e^{-i(\omega t - kx)}}$$

↓
wave function.

$\psi(r, t)$ is called the wave function of the particle or system which describes the space-time behaviour of the particle or system. It helps to obtain every information about the particle.

Wave function for a moving particle



Let m be the mass of the particle which is moving along x -axis with a velocity v_x . Let P_x and E_x represents its momentum and energy respectively.

The wave associated with this particle is a plane wave and it is represented as

$$\psi(x, t) = A e^{-i(\omega t - kx)}$$

$$= A e^{-i\left(\frac{E_x}{\hbar} t - \frac{P_x}{\hbar} x\right)}$$

$$\therefore E = \hbar \omega = \frac{h}{2\pi} \cdot 2\pi \omega$$

$$= \hbar \omega$$

$$\text{or } \omega = \frac{E}{\hbar}$$

$$\lambda = \frac{h}{p} \quad \text{or } \frac{\lambda}{2\pi} = \frac{h}{2\pi p}$$

$$\text{or } \frac{1}{k} = \frac{\hbar}{p}$$

$$\text{or } k = \frac{p}{\hbar}$$

Imp

Schrodinger wave equation :

(i) Time dependent Schrodinger wave equation

Let us consider a particle is moving along x -axis. Let its mass be m and velocity be v_x respectively. Let the momentum of the particle be P_x and total energy be E . The total energy

$$E = K.E + P.E$$

$$E = \frac{p^2}{2m} + V \quad \text{--- (1)}$$

Multiplying by $\psi(x, t)$, we get,

$$E\psi(x, t) = \frac{p^2}{2m} \psi(x, t) + V\psi(x, t) \quad \text{--- (2)}$$

(Now, the wave function for such particle be written as

$$\psi(x, t) = A e^{-i\left(\frac{E}{\hbar}t - \frac{p_x}{\hbar}x\right)} \quad \text{--- (A)}$$

Differentiating it w.r.t 't', we get.

$$\frac{d\psi(x, t)}{dt} = \frac{-i}{\hbar} E \left(A e^{-i\left(\frac{E}{\hbar}t - \frac{p_x}{\hbar}x\right)} \right)$$

$$\frac{d\psi(x, t)}{dt} = -i \times \frac{i}{\hbar} E \psi(x, t)$$

$$\frac{d\psi(x, t)}{dt} = \frac{E}{i\hbar} \psi(x, t)$$

$$\text{or, } E \psi(x, t) = i\hbar \frac{d\psi(x, t)}{dt} \quad \text{--- (3)}$$

diff. eqn (A) w.r.t 'x' we get

$$\frac{d\psi(x, t)}{dx} = \frac{i p_x}{\hbar} A e^{-i\left(\frac{E}{\hbar}t - \frac{p_x}{\hbar}x\right)}$$

Again diff w.r.t. 'x', we get

$$\frac{d^2\psi(x, t)}{dx^2} = \left(\frac{i p_x}{\hbar}\right)^2 \psi(x, t)$$

$$\text{Or } \frac{d^2 \psi(x,t)}{dx^2} = -\frac{p_x^2}{\hbar^2} \psi(x,t)$$

Dividing by $2m$, we get:

$$\frac{1}{2m} \frac{d^2 \psi(x,t)}{dx^2} = -\frac{p_x^2}{2m \hbar^2} \psi(x,t)$$

$$\text{or, } \frac{p_x^2}{2m} \psi(x,t) = -\frac{\hbar^2}{2m} \frac{d^2 \psi(x,t)}{dx^2} \quad \text{--- (4)}$$

Using eqⁿ (3) in (1), we get

$$i\hbar \frac{d\psi(x,t)}{dt} = -\frac{\hbar^2}{2m} \frac{d^2 \psi(x,t)}{dx^2} + V \psi(x,t)$$

$$i\hbar \frac{d\psi}{dt} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \right) \psi$$

$$\Rightarrow \boxed{E\psi = H\psi}$$

where,

$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V$ is called Hamiltonian, i.e., also called total energy operator.

If the particle is free i.e. $V=0$

$$i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} \quad (10)$$

In 3D, it reduces to

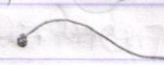
$$i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \left(\frac{d^2 \psi}{dx^2} + \frac{d^2 \psi}{dy^2} + \frac{d^2 \psi}{dz^2} \right)$$

$$\text{or, } i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \nabla^2 \psi \quad (3D)$$

Including PE in 3D, SE can be

$$i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi.$$

② Time independent Schrodinger wave equation.

$\psi(x,t) = \psi(x) e^{-i\omega t}$ $v \rightarrow$ wave velocity
 x -axis

$v = \frac{\omega}{k}$ $v_x \rightarrow$ particle velocity

$$\psi(x,t) = A e^{-i(kx - \omega t)}$$

Let us consider a particle having mass 'm' moving with velocity v_x along x -axis. Accⁿ to de Broglie principle the wave is associated with the particle, its velocity is called wave velocity. Let $\psi(x,t) = A e^{-i(kx - \omega t)}$ be the wave function used to represent the motion of particle.

We have,

wave eqⁿ

$$\left[\frac{d^2\psi}{dx^2} + \frac{1}{v^2} \frac{d^2\psi}{dt^2} \right] = 0 \quad \text{--- (1)}$$

Now,

$$\frac{d\psi}{dt} = -i\omega \psi.$$

$$\Rightarrow \frac{d^2\psi}{dt^2} = (-i\omega)^2 \psi$$

$$\text{or, } \frac{d^2 \psi}{dt^2} = -\omega^2 \psi \quad \text{--- (2)}$$

Again,

$$\frac{d\psi}{dx} = i\kappa \psi$$

$$\Rightarrow \frac{d^2 \psi}{dx^2} = (i\kappa)^2 \psi$$

$$\text{or, } \frac{d^2 \psi}{dx^2} = -\kappa^2 \psi \quad \text{--- (3)}$$

using eqⁿ (2) in (1), we get

$$\frac{d^2 \psi}{dx^2} = -\frac{\omega^2}{v^2} \psi$$

$$\text{since, } \frac{\omega}{v} = \kappa$$

$$\text{or, } \frac{d^2 \psi}{dx^2} = -\kappa^2 \psi$$

$$\text{or, } \frac{d^2 \psi}{dx^2} = -\frac{p^2}{\hbar^2} \psi \quad [\because p = \hbar \kappa]$$

$$\text{Also, } E = \frac{p^2}{2m} + V$$

$$\text{or, } \frac{p^2}{2m} = E - V \quad \text{or, } p^2 = 2m(E - V)$$

$$\text{or, } \frac{d^2 \psi}{dx^2} = -\frac{2m(E - V)}{\hbar^2} \psi$$

$$\text{or, } \left[\frac{d^2 \psi}{dx^2} + \frac{2m(E - V)}{\hbar^2} \psi \right] = 0 \quad \text{(1a)}$$

In 3d, it becomes

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

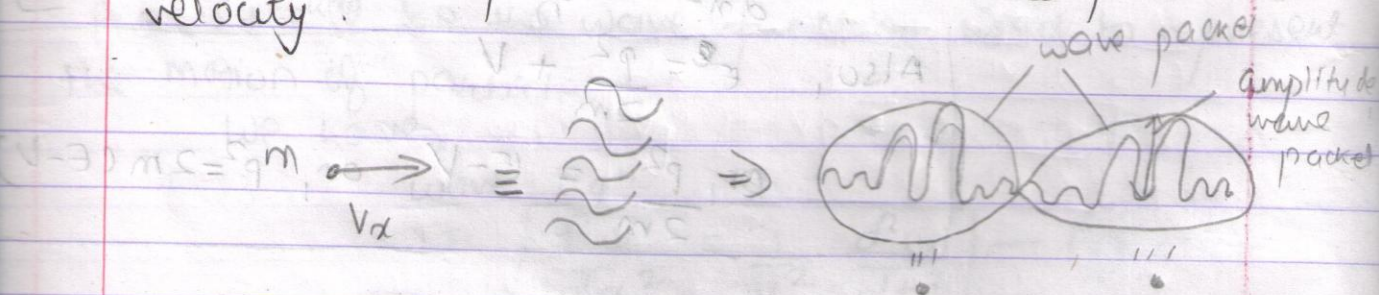
for free particle $V=0$ then

$$\nabla^2 \psi + \frac{2m}{\hbar^2} E \psi = 0$$

Wave packet.

→ Acc to de Broglie principle, each moving particle has wave nature so the particle can be represented by the group of wave. These group of wave when travel in a medium superimpose each other and construct a pattern is called wave packet.

The velocity of the group of wave is called group velocity. The velocity with which the amplitude of the wave packet moves is called particle velocity.



★ Relation between group velocity and ^{phase or wave} particle velocity

Let

$$y_1 = a \sin(\omega t - kx) \text{ and } y_2 = a \sin\{(\omega + \Delta\omega)t - (k + \Delta k)x\}$$

be the two waves used to represent a moving particle
Then accⁿ to superposition principle.

$$y = y_1 + y_2$$

$$\text{or, } y = a \sin(\omega t - kx) + a \sin\{(\omega + \Delta\omega)t - (k + \Delta k)x\}$$

$$= 2a \sin \left[\frac{(\omega t - kx) + \{(\omega + \Delta\omega)t - (k + \Delta k)x\}}{2} \right]$$

$$\cos \left[\frac{(\omega t - kx) - \{(\omega + \Delta\omega)t - (k + \Delta k)x\}}{2} \right]$$

$$= 2a \sin \left\{ \frac{2\omega t + \Delta\omega t}{2} - \frac{2kx + \Delta kx}{2} \right\}$$

$$\cos \left(\frac{\Delta kx - \Delta\omega t}{2} \right)$$

$$y = 2a \sin(\omega t - kx) \cos \left(\frac{\Delta kx - \Delta\omega t}{2} \right)$$

$$\text{or, } y = \left[2a \cos \left(\frac{\Delta kx - \Delta\omega t}{2} \right) \right] \sin(\omega t - kx)$$

This shows that the amplitude of the resulting wave varies with distance and time. This also shows that the amplitude has wave vector $\frac{\Delta k}{2}$ and angular frequency $\frac{\Delta\omega}{2}$.

Now, $\frac{\Delta\omega/2}{\Delta k/2} = \frac{\Delta\omega}{\Delta k} = \frac{d\omega}{dk} = v_g$ is called group velocity

Thus, the group velocity be defined as the rate of change in wave vector with angular velocity.

We have,

$$v_p = \frac{\omega}{k}$$

$$\text{or, } \omega = v_p k$$

Differentiating it w.r.t. k , we get

$$\frac{d\omega}{dk} = v_p + k \frac{dv_p}{dk}$$

$$\begin{aligned} \text{or, } \frac{d\omega}{dk} &= v_p + k \frac{dv_p}{d\lambda} \cdot \frac{d\lambda}{dk} \left[\lambda = \frac{2\pi}{k} \right] \\ &= v_p + k \frac{dv_p}{d\lambda} \cdot \left(-\frac{2\pi}{k^2} \right) \left[\frac{d\lambda}{dk} = -\frac{2\pi}{k^2} \right] \end{aligned}$$

$$\text{or, } \frac{d\omega}{dk} = v_p - \frac{2\pi}{k} \left(\frac{dv_p}{d\lambda} \right)$$

$$\text{or, } \boxed{v_g = v_p - \lambda \frac{dv_p}{d\lambda}} \text{ which is reqd. relation.}$$

Special cases.

- ① If the phase velocity doesn't vary with the wavelength of wave.

$$\text{i.e. } \frac{dv_p}{d\lambda} = 0$$

Eg. velocity of sound in a medium

Then, $v_g = v_p$

i.e. group velocity = phase velocity (i.e. wave velocity)

such a medium is called non-dispersive medium

2) If the phase velocity vary with the wavelength of the wave

i.e. $\frac{dv_p}{d\lambda} \neq 0$. eg. velocity of light in medium (i.e. different colour of light has different velocity)

Then,

$$v_g < v_p.$$

i.e. group velocity < phase velocity (i.e. wave velocity)

such a medium is called dispersive medium.

Questions.

① Show that $\psi(x,t) = A \cos(kx - \omega t)$ can not be used for the wave function for a free particle.

② If $\psi_1(x,t)$ and $\psi_2(x,t)$ are both the soln of time dependent SWE for a particle moving with a potential V . Then prove that the linear combination

$\psi(x,t) = A_1 \psi_1(x,t) + A_2 \psi_2(x,t)$ be also the solⁿ of SWE.

① $\rightarrow$ we have,

Schrodinger wave equation for free particle as

$$i\hbar \frac{d\psi(x,t)}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\psi(x,t)}{dx^2}; v=0.$$

$$\text{L.H.S} = i\hbar \frac{d\psi(x,t)}{dt} = i\hbar A \frac{d(\cos(kx-\omega t))}{dt}$$

$$= i\hbar \omega A \sin(kx-\omega t)$$

$$\begin{aligned} \text{R.H.S} &= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \{A \cos(kx-\omega t)\} \\ &= \frac{\hbar^2}{2m} k^2 A \cos(kx-\omega t) \end{aligned}$$

$\Rightarrow \text{L.H.S} \neq \text{R.H.S.}$

Hence, $\psi(x,t) = A \cos(kx-\omega t)$ can't represent the wave function for a free particle.

② Solⁿ:

Schrodinger wave eqⁿ

$$i\hbar \frac{d\psi(x,t)}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\psi(x,t)}{dx^2} + v\psi(x,t) \quad \text{--- (1)}$$

Since $\psi_1(x,t)$ and $\psi_2(x,t)$ are the solⁿs of SWE then, it must satisfy it

$$\text{then, } i\hbar \frac{d\psi_1(x,t)}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\psi_1(x,t)}{dx^2} + v\psi_1(x,t) \quad \text{--- (2)}$$

$$\text{and, } i\hbar \frac{d\psi_2(x,t)}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\psi_2(x,t)}{dx^2} + v\psi_2(x,t) \quad \text{--- (3)}$$

Multiplying eqⁿ (2) by A_1 and (3) by A_2 and adding then, we get

$$i\hbar \frac{d}{dt} \{A_1 \psi_1(x,t)\} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \{A_1 \psi_1(x,t)\} + V \{A_1 \psi_1(x,t)\}$$

$$i\hbar \frac{d}{dt} \{A_2 \psi_2(x,t)\} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \{A_2 \psi_2(x,t)\} + V \{A_2 \psi_2(x,t)\}$$

$$i\hbar \frac{d}{dt} \{A_1 \psi_1(x,t) + A_2 \psi_2(x,t)\} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \{A_1 \psi_1(x,t) + A_2 \psi_2(x,t)\} + V \{A_1 \psi_1(x,t) + A_2 \psi_2(x,t)\}$$

$$\Rightarrow i\hbar \frac{d}{dt} \psi(x,t) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x,t) + V \psi(x,t) \text{ where,}$$

$$\psi(x,t) = A_1 \psi_1(x,t) + A_2 \psi_2(x,t)$$

This shows that the linear combination of solⁿs $\psi_1(x,t)$ and $\psi_2(x,t)$ are also the solⁿ of SWE.

★ Physical significance of $\psi(x,t)$ and Normalization

Physical significance

→ There is no direct physical meaning with the complex quantity wave function. But when it is taken in the form as $\psi(x,t) \psi^*(x,t) = |\psi(x,t)|^2$ it has a physical meaning it represents probability of finding the particle per unit length for 1D wave function or prob. per unit volume in 3D wave function.

Thus, the entire prob. of finding the particle in a specified region be obtained by

$$\int_a^b |\psi(x,t)|^2 dx \quad \dots \dots \dots \infty$$

$$\int_0^a \int_0^b \int_0^c \psi(x,y,z,t) \psi^*(x,y,z,t) dx dy dz.$$

$$\int_V \psi(\vec{r},t) \psi^*(\vec{r},t) dV \quad \text{--- (3D dimensional)}$$

Further more, characteristics of ψ is as follows

- ① It is a single valued continuous function.
- ② Its value varies at $\pm\infty$.
- ③ Its 1st order and 2nd order differential value is also finite and continuous.

Normalization.

It is the technique of obtaining the exact value of the wave function which is the solution of the given system. Since S.W.E. is linear in form, so it can have many solutions, the exact value of its soln is obtained using this procedure.

Eg :

$$\psi(x,t) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}; \text{ It is normalized wave function.}$$

$$\psi(x,t) = A \sin \frac{n\pi x}{a}; \text{ It is unnormalized wave function}$$

If the wave function is normalized.

$$\int_{-\infty}^{\infty} \psi(x,t) \psi^*(x,t) dx = 1.$$

If the wave function is unnormalized, then it is multiplied by a constant say A as $A \psi(x,t)$

Using normalizing condition, we can write.

$$\int_{-\infty}^{\infty} A \psi(x,t) A^* \psi^*(x,t) dx = 1$$

$$\text{or, } |A|^2 \int_{-\infty}^{\infty} \psi(x,t) \psi^*(x,t) dx = 1$$

$$\text{or, } |A|^2 = \frac{1}{\int_{-\infty}^{\infty} \psi(x,t) \psi^*(x,t) dx}$$

$$\Rightarrow A = \frac{1}{\sqrt{\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx}}$$

$$\sqrt{\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx}$$

Thus, the normalized wave function becomes

$$A \psi(x, t) = \left\{ \frac{1}{\sqrt{\int_{-\infty}^{\infty} |\psi(x, t)|^2 dx}} \right\} \psi(x, t)$$

Q5) Normalize the following wave function.

$$\psi(x, t) = N e^{i(kx - \omega t)} \quad ; -1 \leq x \leq 1$$

→ Soln:

Normalized wave function is

$$\int_{-\infty}^{\infty} \psi(x, t) \cdot \psi^*(x, t) dx = 1$$

For this case,

$$\int_{-1}^1 N e^{i(kx - \omega t)} \cdot N^* e^{-i(kx - \omega t)} dx = 1$$

$$N^2 \int_{-1}^1 |e^{i(kx - \omega t)}|^2 dx = 1$$

$$N = \frac{1}{\sqrt{\int_{-1}^1 e^{2ikx - 2i\omega t} dx}}$$

$$\psi(x, t) = \frac{1}{\sqrt{2ik [e^{2ikx - 2i\omega t}]_{-1}^1}}$$

$$N^2 \psi(x,t) = \frac{1}{\sqrt{2}}$$

$$\text{or } |N|^2 \int_{-1}^1 dx = 1$$

$$\text{or } N^2 [x]_{-1}^1 = 1$$

$$N^2 [2] = 1$$

$$N = \frac{1}{\sqrt{2}}$$

The normalized wave function becomes

$$\psi(x,t) = \frac{1}{\sqrt{2}} e^{i(kx - \omega t)}$$

$$(2) \quad \psi_n = A \frac{\sin n\pi x}{a}; \quad 0 < x < a$$

→ Solⁿ 0

According to rule for normalization

$$\int_{-\infty}^{\infty} \psi^* \psi dx = 1$$

$$\int_0^a A^* \frac{\sin n\pi x}{a} \cdot A \frac{\sin n\pi x}{a} dx = 1$$

$$A^2 \int_0^a \frac{\sin^2 n\pi x}{a} dx = 1$$

NOTE: $\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}$

$$A^2 \frac{1}{2} \int_0^a \left(1 - \cos \frac{2n\pi x}{a} \right) dx = 1$$

$$A^2 \times \frac{1}{2} \left(x - \left(\frac{\sin 2n\pi x}{a} \right) \times \frac{a}{2n\pi} \right)_0^a = 1$$

$$A^2 \times \frac{1}{2} \left(a - \left(\frac{\sin 2n\pi a}{a} \right) \times \frac{a}{2n\pi} \right) = 1$$

$$A^2 \times \frac{1}{2} \left(a - \sin 2n\pi \times \frac{a}{2n\pi} \right) = 1$$

$$A^2 \times \frac{1}{2} (a - 0) = 1$$

$$A^2 = \frac{2}{a}$$

$$A = \sqrt{\frac{2}{a}}$$

$\therefore$ The normalized wave function is

$$\psi(x,t) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

③ Normalize the following 1D wave function
 $\psi(x) = A e^{-x^2/2}$ betⁿ $-\infty$ to ∞

$\rightarrow$ Solⁿ:

$$\psi(x) = A e^{-x^2/2}$$

Acc. to rule for normalization

$$\int_{-\infty}^{\infty} \psi^* \psi dx = 1$$

$$\int_{-\infty}^{\infty} A^2 e^{-x^2} dx = 1$$

$$A^2 \int_{-b}^b e^{-2x^2/2} dx = 1$$

$$A^2 \int_{-b}^b e^{-x^2} dx = 1$$

$$A^2 \sqrt{\frac{\pi}{1}} = 1$$

$$A^2 = \frac{1}{\sqrt{\pi}}$$

$$A = (\pi^{-1/2})^{1/2}$$

$$A = \pi^{-1/4}$$

∴ The normalized wave function is

$$\psi(x,t) = \pi^{-1/4} e^{-x^2/2}$$

④ Normalize the wave function

$\psi(x) = A(\sin x + i \cos x)$ in the region $-1 \leq x \leq 1$.

→ Here,

$$\psi(x) = A(\sin x + i \cos x)$$

Acc. to rule for normalization,

$$\int_{-\infty}^{\infty} \psi^* \psi dx = 1$$

$$\text{or, } \int_{-1}^1 A^* (\sin x - i \cos x) A (\sin x + i \cos x) dx = 1$$

$$\text{or, } A^2 \int_{-1}^1 (\sin^2 x + \cos^2 x) dx = 1$$

$$\text{or, } A^2 \int_{-1}^1 dx = 1$$

$$\text{or, } A^2 [x]_{-1}^1 = 1$$

$$\text{or, } A^2 \times 2 = 1$$

$$\text{or, } A = \frac{1}{\sqrt{2}}$$

$\therefore$ The normalized wave function is

$$\psi(x, t) = \frac{1}{\sqrt{2}} (\sin x + i \cos x)$$

(5) Normalize the following
 $\psi(x) = A e^{i a x} e^{-b t}$; L_1 to L_2

$\Rightarrow$ Solⁿ :

According to rule for normalization,

$$\int_{-\infty}^{\infty} \psi^* \psi dx = 1$$

$$\int_{L_1}^{L_2} A^* e^{-i a x - b t} \cdot A e^{i a x - b t} dx = 1$$

$$A^2 \int_{L_1}^{L_2} e^{-i a x - b t + i a x - b t} dx = 1$$

$$A^2 \int_{L_1}^{L_2} e^{-2 b t} dx = 1$$

$$A^2 e^{-2bt} [x]_{L_1}^{L_2} = 1$$

$$A^2 e^{-2bt} [L_2 - L_1] = 1$$

$$A = \frac{1}{\sqrt{e^{-2bt} [L_2 - L_1]}}$$

∴ The normalized eqⁿ is

$$\psi(x) = \frac{1}{\sqrt{e^{-2bt} (L_2 - L_1)}} e^{i(ax - bt)}$$

⑥ A particle is represented by (at $t=0$) by the wave function on

$$\psi(x,t) = \begin{cases} A(a^2 - x^2) & \text{if } -a \leq x \leq a \\ 0 & \text{otherwise.} \end{cases}$$

Find A.

→ Solⁿ:

Acc. to rule for normalization,

$$\int_{-\infty}^{\infty} \psi^* \psi dx = 1$$

$$\int_{-a}^a A^* (a^2 - x^2) A (a^2 - x^2) dx = 1$$

$$A^2 \int_{-a}^a [(a^2 - x^2)(a^2 - x^2)] dx = 1$$

$$\text{or, } A^2 \int_{-a}^a [a^4 - a^2 x^2 - a^2 x^2 + x^4] dx = 1$$

$$\text{or, } A^2 \int_{-a}^a [a^4 - 2a^2 x^2 + x^4] dx = 1$$

$$A^2 \left[a^4 \left(x \right)_{-a}^a - 2a^2 \left(\frac{x^3}{3} \right)_{-a}^a + \left(\frac{x^5}{5} \right)_{-a}^a \right] = 1$$

$$A^2 \left[a^4 \pi 2a - 2a^2 \pi \left(\frac{a^3}{3} + \frac{a^3}{3} \right) + \frac{2a^5}{5} \right] = 1$$

$$A^2 \left[2a^5 - \frac{4a^5}{3} + \frac{2a^5}{5} \right] = 1$$

$$A^2 \left[\frac{30a^5 - 20a^5 + 6a^5}{15} \right] = 1$$

$$A^2 \pi \frac{16a^5}{15} = 1$$

$$A = \frac{\sqrt{15a^5}}{\sqrt{16a^5}} = \frac{1}{4} \sqrt{\frac{15}{a^5}}$$

∴ The normalized funcⁿ is

$$\psi(r, t) = \frac{1}{4} \sqrt{\frac{15}{a^5}} (a^2 - x^2)$$

⑦ Normalize.

① $\phi(r) = (1 + i^2 x) ; 0 \leq x \leq 1$

→ Acc. to rule for normalization,

$$\int_{-\infty}^{\infty} \phi^* \phi \, dx = 1.$$

$$\int_0^1 A^* (1 - ix) A (1 + ix) \, dx = 1$$

$$A^2 \int_0^1 (1 - i^2 x^2) \, dx = 1$$

$$A^2 \int_0^1 (1 + x^2) \, dx = 1.$$

$$A^2 \left[x + \frac{x^3}{3} \right]_0^1 = 1$$

$$A^2 \left[1 + \frac{1}{3} \right] = 1$$

$$A^2 \times \frac{4}{3} = 1 \quad \star$$

$$\therefore A = \frac{\sqrt{3}}{2}$$

The normalized funcⁿ is

$$\phi(x, t) = \frac{\sqrt{3}}{2} (1 + ix)$$

(ii) $\psi(x) = A e^{-x^2/2}$

→ Acc. to rule for normalization,

$$\int_{-\infty}^{\infty} \psi^* \psi dx = 1$$

$$\int_{-\infty}^{\infty} A^* (e^{-x^2/2}) \cdot A (e^{-x^2/2}) dx = 1$$

$$A^2 \int_{-\infty}^{\infty} (e^{-x^2}) dx = 1$$

$$A^2 \pi \sqrt{\pi} = 1$$

$$A = (\pi)^{-1/4}$$

The normalized wave eqⁿ is

$$\psi(x,t) = (\pi)^{-1/4} \cdot e^{-x^2/2}$$

★ Expectation in Quantum mechanics.

The expectation value of a dynamical variable in quantum mechanics is the average value of the possible measurement.

Dynamical variable :- The physical quantity whose value changes with the displacement and time is called dynamical variable.

Mathematically, the expectation ^{value} ~~variable~~ of a dynamical

dynamical variable A is defined by.

$$\langle A \rangle = \int \psi^* \hat{A} \psi dx$$

where $\hat{A}$ $\rightarrow$ operator respective to the dynamical variable A .

Eg position.

$$\langle x \rangle = \int \psi^* \hat{x} \psi dx$$

$$\langle x \rangle = \int \psi^*(x) x \psi(x) dx$$

$$\Rightarrow \langle y \rangle = \int \psi^*(y) \hat{y} \psi(y) dy$$

$$\Rightarrow \langle z \rangle = \int \psi^*(z) \hat{z} \psi(z) dz$$

Momentum

$$\langle p \rangle = \int \psi^* \hat{p} \psi dx$$

$$= \int \psi^* (-i\hbar \nabla) \psi dx$$

where, $\hat{p} = -i\hbar \nabla$.

$$\langle p_x \rangle = \int \psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \psi dx ; \hat{p}_x = -i\hbar \frac{\partial}{\partial x}$$

$$\langle p_y \rangle = \int \psi^* \left(-i\hbar \frac{\partial}{\partial y} \right) \psi dy ; \hat{p}_y = -i\hbar \frac{\partial}{\partial y}$$

$$\langle p_z \rangle = \int \psi^* \left(-i\hbar \frac{\partial}{\partial z} \right) \psi dz ; \hat{p}_z = -i\hbar \frac{\partial}{\partial z}$$

Qs) Find the expectation value for energy within the boundary $-1 \leq x \leq 1$ for the wave function $\psi(x) = N e^{i(kx - \omega t)}$.

→ Soln:

Acc. to rule for normalization.

$$\int_{-\infty}^{\infty} \psi^* \psi dx = 1$$

$$\text{or, } \int_{-1}^1 N^* e^{-i(kx - \omega t)} N e^{i(kx - \omega t)} dx = 1$$

$$\text{or, } N^2 \int_{-1}^1 e^{-ikx + i\omega t + ikx - i\omega t} dx = 1$$

$$N^2 \int_{-1}^1 1 dx = 1$$

$$N^2 [x]_{-1}^1 = 1$$

$$N^2 \times 2 = 1$$

$$N = \frac{1}{\sqrt{2}}$$

∴ The normalized wave function becomes

$$\psi(x) = \frac{1}{\sqrt{2}} e^{i(kx - \omega t)}$$

Now, the expectation value for energy is obtained as

$$\langle E \rangle = \int \psi^* \hat{E} \psi dx$$

$$= \int_{-1}^1 \frac{1}{\sqrt{2}} e^{-ickx - \omega t} \cdot i\hbar \frac{\partial}{\partial t} \left(\frac{1}{\sqrt{2}} e^{ickx - \omega t} \right) dx$$

where, $\hat{E} = i\hbar \frac{\partial}{\partial t}$

$$\langle E \rangle = \frac{i\hbar}{2} \int_{-1}^1 e^{-ickx - \omega t} e^{ickx - \omega t} (i\omega) dx$$

$$\langle E \rangle = \frac{-i^2 \hbar \omega}{2} \int_{-1}^1 e^0 dx$$

$$\langle E \rangle = \frac{\hbar \omega \times 2}{2}$$

$$\langle E \rangle = \hbar \omega$$

Q. Find the energy expectation value of a particle described by the wave function $\psi(x) = Ae^{iax - bt}$ moving betⁿ x_1 to x_2 .

→ Solⁿ:

Acc. to scale for normalization

$$\int_{-\infty}^{\infty} \psi^* \psi dx = 1$$

$$\int_{L_1}^{L_2} A^* e^{-i\alpha x - bt} \cdot A e^{i\alpha x - bt} dx = 1$$

$$A^2 \int_{L_1}^{L_2} e^{-i\alpha x - bt + i\alpha x - bt} dx = 1$$

$$A^2 \int_{L_1}^{L_2} e^{-2bt} dx = 1$$

$$A^2 e^{-2bt} [L_2 - L_1] = 1$$

$$A = \frac{1}{\sqrt{e^{-2bt} [L_2 - L_1]}}$$

The normalized wave function becomes

$$\psi(x) = \frac{1}{\sqrt{e^{-2bt} [L_2 - L_1]}} \cdot e^{i\alpha x - bt}$$

Now, the expectation value for energy is obtained as

$$\langle E \rangle = \int \psi^* \hat{E} \psi dx$$

$$\langle E \rangle = \int_{L_1}^{L_2} A^* e^{-i\alpha x - bt} \cdot \left(i\hbar \frac{d}{dt} (A e^{i\alpha x - bt}) \right) dx$$

$$= A^2 i\hbar \int_{L_1}^{L_2} e^{-i\alpha x - bt} \cdot (-b) e^{i\alpha x - bt} dx$$

$$= A^2 (-b i\hbar) \int_{L_1}^{L_2} e^{-i\alpha x - bt + i\alpha x - bt} dx$$

$$= A^2 (-b i\hbar) \cdot e^{-2bt} \int_{L_1}^{L_2} dx$$

$$= A^2 (-b i\hbar) \cdot e^{-2bt} \cdot [L_2 - L_1]$$

$$= \frac{1}{e^{-2bt} \cdot [L_2 - L_1]} \cdot A^2 (-b i\hbar) \cdot e^{-2bt} [L_2 - L_1]$$

$$\therefore \langle E \rangle = -i\hbar b$$

Qs) Find the average value of P and P^2 for the wave function $\psi(x) = \sqrt{\frac{2}{l}} \sin \frac{\pi x}{l}$ for region $0 < x < l$.

→ Solⁿ :-

The expectation value for P is obtained as

$$\langle P \rangle = \int \psi^* \left(-i\hbar \frac{d}{dx} \right) \psi dx$$

$$= \int_0^l \sqrt{\frac{2}{l}} \sin \frac{\pi x}{l} \left(-i\hbar \frac{d}{dx} \sqrt{\frac{2}{l}} \sin \frac{\pi x}{l} \right) dx$$

$$= \frac{2}{l} \int_0^l \sqrt{\frac{\sin \pi x}{l}} \left(-i\hbar \frac{d}{dx} \sqrt{\frac{\sin \pi x}{l}} \right) dx$$

$$= \frac{2(-i\hbar)}{l} \int_0^l \sqrt{\frac{\sin \pi x}{l}} \left(\frac{1}{2} \times \frac{1}{\sqrt{\sin \pi x}} \times \cos \frac{\pi x}{l} \times \frac{\pi}{l} \right) dx$$

$$= -\frac{2i\hbar}{l} \times \frac{\pi}{l} \int_0^l \cos \frac{\pi x}{l} dx$$

$$= -\frac{2i\hbar \pi}{l^2} \left(\sin \frac{\pi x}{l} \right)_0^l$$

$$= -\frac{2i\hbar}{l} \cdot \sin \frac{\pi x}{l}$$

$$= -\frac{2i\hbar}{l} \times 0$$

$$\hat{p} = -i\hbar \frac{d}{dx}$$

$$\hat{p}^2 = -\hbar^2 \frac{d^2}{dx^2}$$

$$\langle p^2 \rangle = \int \psi^* \left(-\hbar^2 \frac{d^2}{dx^2} \right) \psi dx$$

$$= \int_0^l \sqrt{\frac{2}{l}} \sin \frac{\pi x}{l} \left(-\hbar^2 \frac{d^2}{dx^2} \right) \sqrt{\frac{2}{l}} \sin \frac{\pi x}{l} dx$$

$$= -\frac{2\hbar^2}{l} \int_0^l \sin \frac{\pi x}{l} \left(\frac{\pi^2}{l^2} \right) \left(-\sin \frac{\pi x}{l} \right) dx$$

$$= \frac{2\hbar^2}{l} \times \frac{\pi^2}{l^2} \int_0^l \left(\sin^2 \frac{\pi x}{l} \right) dx$$

$$= \frac{2\hbar^2}{l^3} \times \pi^2 \int_0^l \left(\frac{1 - \cos \frac{2\pi x}{l}}{2} \right) dx$$

$$= \frac{\pi^2 \hbar^2}{l^3} \left(x - \frac{\sin \frac{2\pi x}{l}}{\frac{2\pi}{l}} \right)_0^l$$

$$= \frac{\pi^2 \hbar^2}{l^3} \cdot l$$

$$= \frac{\pi^2 \hbar^2}{l^2}$$

$$= \frac{\pi^2 \hbar^2}{l^2}$$

Qs) Find the expectation value of momentum m for the wave function $\phi(x) = (1+ix)$ within the region of $0 \leq x \leq 1$.

→ Soln

The normalized wave function is

$$\phi(x) = \frac{\sqrt{3}}{2} (1+ix)$$

The expectation value for P is obtained as

$$\langle P \rangle = \int \phi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \phi dx$$

$$= \int_0^1 \frac{\sqrt{3}}{2} (1-ix) \left(-i\hbar \frac{\partial}{\partial x} \right) \frac{\sqrt{3}}{2} (1+ix) dx$$

$$= \frac{3}{4} \int_0^1 (1-ix) \left(-i\hbar \frac{d}{dx} (1+ix) \right) dx$$

$$= \frac{3}{4} (-i\hbar) \int_0^1 (1-ix) (i) dx$$

$$= (-i\hbar) \frac{3}{4} \int_0^1 (i - i^2 x) dx$$

$$= -i\hbar \frac{3}{4} \int_0^1 (i + x) dx$$

$$= -i\hbar \frac{3}{4} \left(ix + \frac{x^2}{2} \right) \Big|_0^1$$

$$= -i\hbar \times \frac{3}{4} \left(i + \frac{1}{2} \right) dx$$

$$= -i\hbar \times \frac{3}{4} \times \frac{(2i+1)}{2} dx$$

$$= \frac{3}{8} - i\hbar (2i+1)$$

$$= \frac{3}{8} (-2i^2\hbar - i\hbar)$$

$$= \frac{3}{8} (2\hbar - i\hbar)$$

$$\langle P \rangle = \frac{3\hbar}{8} (2-i)$$

★ Probability current density and eqⁿ of continuity

The equation of continuity states that the rate of decrease in probability density of charge is equal to the rate of flow of charge through the surface enclosing the volume.

$$\frac{dS}{dt} = -\nabla \cdot \vec{J}$$

where S is called probability density
 $\vec{J}$ " " " prob. current density

We have Schrodinger wave equation

$$i\hbar \frac{d\psi}{dt} = \frac{-\hbar^2}{2m} \nabla^2 \psi + V\psi \quad \text{--- (1)}$$

Taking complex conjugate, we get,

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi^* + V \psi^* \quad \text{--- (2)}$$

Subtracting eqⁿ (2) from (1), we get.

$$i\hbar \frac{d\psi}{dt}$$

Multiplying eqⁿ (1) by ψ^* and eqⁿ (2) by ψ from left, and subtracting eqⁿ (2) from (1), we get

$$i\hbar \psi^* \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \psi^* \nabla^2 \psi + \psi^* V \psi$$

$$\begin{array}{ccc} -i\hbar \psi \frac{d\psi^*}{dt} & = & -\frac{\hbar^2}{2m} \psi \nabla^2 \psi^* + \psi V \psi^* \\ (+) & & (+) \quad \quad (-) \end{array}$$

$$i\hbar \left(\psi^* \frac{d\psi}{dt} + \psi \frac{d\psi^*}{dt} \right) = -\frac{\hbar^2}{2m} (\psi^* \nabla^2 \psi + \psi \nabla^2 \psi^*)$$

$$\text{or, } i\hbar \frac{d}{dt} (\psi^* \psi) = -\frac{\hbar^2}{2m} (\nabla \psi^* \nabla \psi + \psi^* \nabla^2 \psi - \nabla \psi^* \nabla \psi - \psi \nabla^2 \psi^*)$$

$$\text{or, } \frac{d}{dt} (\psi^* \psi) = -\frac{\hbar}{2im} \nabla (\psi^* \nabla \psi - \psi \nabla \psi^*)$$

$$\text{or, } \frac{d}{dt} (\psi^* \psi) = -\nabla \left(\frac{\hbar}{2im} (\psi^* \nabla \psi - \psi \nabla \psi^*) \right)$$

$$\text{Comparing with } \frac{dS}{dt} = -\nabla J$$

where $S = \psi^* \psi$ is called prob. density

$J = \frac{\hbar}{2im} (\psi^* \nabla \psi - \psi \nabla \psi^*)$ is called prob. current density.

$$\text{or, } \frac{dS}{dt} + \nabla \cdot \vec{J} = 0$$

$\therefore$ Proved,,

The prob. current density along x, y and z axis is written as.

$$J_x = \frac{\hbar}{2im} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right)$$

$$J_y = \frac{\hbar}{2im} \left(\psi^* \frac{d\psi}{dy} - \psi \frac{d\psi^*}{dy} \right)$$

and,

$$J_z = \frac{\hbar}{2im} \left(\psi^* \frac{d\psi}{dz} - \psi \frac{d\psi^*}{dz} \right)$$

Questions:

- 1) Show that the prob. current density of real wave function is zero.
- 2) Show that the prob. current density for a free particle is equal to product of velocity and prob. density.

Q.1) For real wave function

$$\psi = \psi^*$$

Then,

probability current density

$$J = \frac{\hbar}{2im} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right)$$

$$= \frac{\hbar}{2im} \times 0$$

$$= 0$$

$\therefore$ Proved

Q2) we have SWE for free particle along x-axis

$$i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \psi$$

$$\boxed{i\hbar \frac{d\psi}{dt} = \frac{P_x^2}{2m}}$$

Again,

$$P_x \psi = -i\hbar \frac{d\psi}{dx}$$

$$\text{or, } \frac{d\psi}{dx} = \frac{P_x}{-i\hbar} \psi$$

Taking complex conjugate, we get,

$$\frac{d\psi^*}{dx} = \frac{P_x}{i\hbar} \psi^* \quad \text{--- (2)}$$

The prob. current density be written as

$$J_x = \frac{\hbar}{2im} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right)$$

$$= \frac{\hbar}{2im} \left(\psi^* \left(\frac{p_x \psi}{-i\hbar} \right) - \psi \left(\frac{p_x \psi^*}{i\hbar} \right) \right)$$

$$= \frac{\hbar}{2im} \left(\frac{2\psi^* p_x \psi}{-i\hbar} \right)$$

$$= \frac{p_x}{m} \psi^* \psi$$

$$= \frac{mv}{m} \psi^* \psi$$

$$= v \psi^* \psi$$

$$= v(\psi)$$

current density = velocity $\times$ prob. density.

Q3 Find the prob. current density of the wave function.

$$\psi(x) = \frac{e^{ikx}}{x}$$

→ Here

$$\psi(x) = \frac{e^{ikx}}{x}$$

$$\psi^*(x) = \frac{e^{-ikx}}{x}$$

$$\frac{d\psi}{dx} = x^{-1} \cdot e^{ikx} = e^{ikx} \left(-\frac{1}{x^2} \right) + \frac{ik}{x} (e^{ikx})$$

$$\frac{d\psi^*}{dx} = x^{-1} \cdot e^{-ikx} = e^{-ikx} \left(-\frac{1}{x^2} \right) + \left(\frac{-ik}{x} \right) (e^{-ikx})$$

$$\frac{d\psi}{dx} = e^{ikx} \left(-\frac{1}{x^2} + \frac{ik}{x} \right)$$

$$\frac{d\psi^*}{dx} = e^{-ikx} \left(-\frac{1}{x^2} - \frac{ik}{x} \right)$$

$$\begin{aligned}
 J_x &= \frac{\hbar}{2im} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right) \\
 &= \frac{\hbar}{2im} \left(\frac{e^{-ikx} \cdot e^{ikx} \left(-\frac{1}{x^2} + \frac{ik}{x} \right) - \frac{e^{ikx} \cdot e^{-ikx} \left(-\frac{1}{x^2} - \frac{ik}{x} \right)}{x} \right) \\
 &= \frac{\hbar}{2im} \left(\frac{1}{x} \left(-\frac{1}{x^2} + \frac{ik}{x} \right) - \frac{1}{x} \left(-\frac{1}{x^2} - \frac{ik}{x} \right) \right) \\
 &= \frac{\hbar}{2im} \left(\frac{1}{x} \left(-\frac{1}{x^2} + \frac{ik}{x} + \frac{1}{x^2} + \frac{ik}{x} \right) \right) \\
 &= \frac{\hbar}{2im} \cdot \frac{2ik}{x^2} \\
 &= \frac{\hbar k}{mx^2} = \frac{p_x}{mx^2} \\
 &= \frac{mv}{mx^2} \\
 &= \frac{v}{x^2}
 \end{aligned}$$

Similarly

$$J_y = \frac{v}{y^2}$$

$$J_z = \frac{v}{z^2}$$

In general, Prob. current density for $\psi(r) = \frac{e^{ikr}}{r}$

$$J = \frac{v}{r^2}$$

Qs) Find the probability current density of the wave function

$\psi(x) = e^{ikx} + Ae^{-ikx}$ in the region where $x < 0$ and potential $V = 0$.

→ Solⁿ :

$$\psi(x) = e^{ikx} + Ae^{-ikx} \quad A = |A|$$

$$\psi^*(x) = e^{-ikx} + Ae^{ikx}$$

$$\frac{d\psi}{dx} = ik e^{ikx} + A(-ik) e^{-ikx}$$

$$= ik e^{ikx} - Aik e^{-ikx}$$

$$\frac{d\psi^*}{dx} = -ik e^{-ikx} + Aik e^{ikx}$$

$$J = \frac{\hbar}{2im} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right)$$

$$= \frac{\hbar}{2im} \left((e^{-ikx} + Ae^{ikx}) (ik e^{ikx} - Aik e^{-ikx}) - (e^{ikx} + Ae^{-ikx}) (-ik e^{-ikx} + Aik e^{ikx}) \right)$$

$$= \frac{\hbar}{2im} \left(ik - Aik e^{2ikx} + Aik e^{2ikx} - A^2 ik - (-ik + Aik e^{-2ikx} - Aik e^{-2ikx} + A^2 ik) \right)$$

$$= \frac{\hbar}{2im} (2ik - 2A^2 ik) = \frac{\hbar}{2im} 2ik (1 - A^2)$$

$$= \frac{\hbar k}{m} (1 - A^2)$$

$$= \frac{\hbar k}{m} - \frac{\hbar k}{m} A^2$$

$$= J_{in} + J_{ref}$$

$$A = 1$$

$$\text{where, } J_{in} = \frac{\hbar k}{m} = v$$

$$\text{and } J_{ref} = -\frac{\hbar k}{m} A^2$$

Operator:

It is a rule which is when operated to the wave function, it changes the function into another wave function.

Types of Operators:

- i) Linear operator
- ii) zero operator
- iii) Singular and Non-singular operator
- iv) Identity operator
- v) Inverse operator
- vi) Parity operator
- vii) Hermitian operator
- viii) Commutation operator
- ix) Eigen value operator

(i) Linear operator

The operators are said to be linear operator if they satisfy the following rules.

$$(a) \hat{A}(\phi_1 + \phi_2) = \hat{A}\phi_1 + \hat{A}\phi_2$$

$$(b) c\hat{A}\phi = \hat{A}c\phi \text{ where } c \text{ is a constant.}$$

(ii) Zero operator

An operator is said to be zero operator which vanishes the wave function after operation.

$$\text{eg. } \hat{A}\psi = 0.$$

(iii) Singular and non-singular operators.

The operator whose inverse can't be defined is called singular operator and the operator whose respective inverse op. can be defined is called non-singular operator.

(iv) Identity operator

$$\hat{A}\psi = \psi$$

The operator resulting no any changes to the wave function is called identity operator.

(v) Inverse operator.

$$\frac{\partial \phi(x)}{\partial x} = \psi(x)$$

$$\int \psi(x) dx = \phi(x)$$

An operator is said to be inverse of ^{with another op} given operator when its result is operated ~~at~~ gives the same wave function.

(v) Eigen value operator

An operator which operates as follows is called eigen value operator, i.e., it results the same wave function multiplied a constant.

The wave function is called eigen value wave function.

$$\psi(m, t) = e^{i\left(\frac{x p_x}{\hbar} - \omega t\right)}$$

Find eigen value of momentum op.

$$\hat{p}_x \psi(m, t) = ?$$

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$$

$$\hat{p}_x \psi(m, t) = -i\hbar \frac{\partial}{\partial x} e^{i\left(\frac{x p_x}{\hbar} - \omega t\right)}$$

$$= -i\hbar \times \frac{i}{\hbar} p_x e^{i\left(\frac{x p_x}{\hbar} - \omega t\right)}$$

$$\hat{p}_x \psi(m, t) = p_x e^{i\left(\frac{x p_x}{\hbar} - \omega t\right)} = p_x \psi(m, t)$$

Hence, p_x is the eigen value.

Establish the eigen value eqⁿ of the operator $\left(\frac{\partial^2}{\partial x^2} - x^2\right)$ if its eigen function is $e^{-x^2/2}$.

→ Solⁿ :

$$\hat{A} \psi = \lambda \psi$$

Here $\hat{A} = \frac{\partial^2}{\partial x^2} - x^2$ $\psi = e^{-x^2/2}$

$$\hat{A} \psi = \left(\frac{\partial^2}{\partial x^2} - x^2 \right) (e^{-x^2/2})$$

$$= \frac{\partial^2}{\partial x^2} (e^{-x^2/2}) - x^2 \cdot e^{-x^2/2}$$

$$= -e^{-x^2/2} + x^2 - x^2 \cdot e^{-x^2/2}$$

$$= x^2 \cdot e^{-x^2/2} - e^{-x^2/2} - x^2 \cdot e^{-x^2/2}$$

$$= -e^{-x^2/2}$$

$$= (-1) e^{-x^2/2}$$

$$\hat{A} \psi = (-1) \psi$$

$$\therefore \text{Eigen value } \lambda = -1$$

VII) Hermitian operator

The operator respective to a dynamical variable whose expectation value is real is called Hermitian operator

$A \rightarrow$ dynamical variation

$\hat{A} \rightarrow$ operator

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi_1^* \hat{A} \psi_2 dx \text{ is real}$$

In another way, Hermitian operator is defined as

$$\int_{-\infty}^{\infty} \psi_1^* \hat{A} \psi_2 dx = \int_{-\infty}^{\infty} (\hat{A} \psi_1)^* \psi_2 dx.$$

Properties of Hermitian operator.

1) The sum of two Hermitian operator is Hermitian.

Proof: Let $\hat{\alpha}$ & $\hat{\beta}$ are the two Hermitian operators. Let ψ_1 and ψ_2 be the two wave

$$\text{then } \int_{-\infty}^{\infty} \psi_1^* \hat{\alpha} \psi_2 dx = \int_{-\infty}^{\infty} (\hat{\alpha} \psi_1)^* \psi_2 dx$$

$$\text{and, } \int_{-\infty}^{\infty} \psi_1^* \hat{\beta} \psi_2 dx = \int_{-\infty}^{\infty} (\hat{\beta} \psi_1)^* \psi_2 dx.$$

then,

$$\int_{-\infty}^{\infty} \psi_1^* (\hat{\alpha} + \hat{\beta}) \psi_2 dx = \int_{-\infty}^{\infty} \psi_1^* \hat{\alpha} \psi_2 dx + \int_{-\infty}^{\infty} \psi_1^* \hat{\beta} \psi_2 dx$$

$$= \int_{-\infty}^{\infty} (\hat{\alpha} \psi_1)^* \psi_2 dx + \int_{-\infty}^{\infty} (\hat{\beta} \psi_1)^* \psi_2 dx$$

$$= \int_{-\infty}^{\infty} \{ (\hat{\alpha} \psi_1)^* + (\hat{\beta} \psi_1)^* \} \psi_2 dx$$

$$= \int_{-\infty}^{\infty} \underbrace{\{(\hat{\alpha} + \hat{\beta})\psi_1\}}^{\text{Hermitian op}}^* \psi_2 dx$$

$\Rightarrow$ Sum of two Hermitian op is Hermitian.

2) The ~~prop~~ product of two Hermitian operator is Hermitian if they commute (i.e. $\hat{\alpha}\hat{\beta} = \hat{\beta}\hat{\alpha}$)

$\Rightarrow$ Proof:

Let ψ_1 and ψ_2 are two wave function and $\hat{\alpha}$ and $\hat{\beta}$ are the two operators respectively.

To show:

$$\int_{-\infty}^{\infty} \psi_1^* (\hat{\alpha}\hat{\beta}) \psi_2 dx = \int_{-\infty}^{\infty} \{(\hat{\alpha}\hat{\beta})\psi_1\}^* \psi_2 dx$$

$$\text{L.H.S} = \int_{-\infty}^{\infty} \psi_1^* (\hat{\alpha}\hat{\beta}) \psi_2 dx = \int_{-\infty}^{\infty} (\hat{\alpha}\psi_1)^* \hat{\beta} \psi_2 dx$$

$$= \int_{-\infty}^{\infty} (\hat{\beta}\hat{\alpha}\psi_1)^* \psi_2 dx$$

Since $\hat{\alpha}$ & $\hat{\beta}$ are Hermitian

$$= \int_{-\infty}^{\infty} (\hat{\alpha}\hat{\beta}\psi_1)^* \psi_2 dx$$

$$= \text{R.H.S.} \quad [\hat{\alpha}\hat{\beta} = \hat{\beta}\hat{\alpha}]$$

3. The eigen values of Hermitian operators are real
Proof: let λ be the eigen value of a Hermitian operator $\hat{A}$ with the wave function ψ .
Then,

$$\hat{A} \psi = \lambda \psi \quad \text{--- (1)}$$

taking complex conjugate, we get,

$$(\hat{A} \psi)^* = (\lambda \psi)^*$$

$$\text{or, } \hat{A}^* \psi^* = \lambda^* \psi^* \quad \text{--- (2)}$$

Now,

$$\int_{-\infty}^{\infty} \psi^* \hat{A} \psi dx = \int_{-\infty}^{\infty} (\hat{A} \psi)^* \psi dx$$

$$\text{or, } \int_{-\infty}^{\infty} \psi^* \lambda \psi dx = \int_{-\infty}^{\infty} \lambda^* \psi^* \psi dx$$

$$\text{or, } \lambda \int_{-\infty}^{\infty} \psi^* \psi dx = \lambda^* \int_{-\infty}^{\infty} \psi^* \psi dx$$

$$\text{Then, } \lambda = \lambda^*$$

$$\left[\because \int_{-\infty}^{\infty} \psi^* \psi dx = 1 \right]$$

4. The two eigen functions of a hermitian op. belonging to two eigen values are orthogonal functions.

Proof: let ψ_1 and ψ_2 are the two wave functions and $\hat{A}$ be the Hermitian op. let λ_1 and λ_2 be their respective eigen values of the operator then

$$\hat{A} \psi_1 = \lambda_1 \psi_1 \quad \hat{A} \psi_2 = \lambda_2 \psi_2$$

Now,

$$\int_{-\infty}^{\infty} \psi_2^* \hat{A} \psi_1 dx = \int_{-\infty}^{\infty} (\hat{A} \psi_2)^* \psi_1 dx$$

$$\text{or, } \int_{-\infty}^{\infty} \psi_2^* \lambda_1 \psi_1 dx = \int_{-\infty}^{\infty} \lambda_2^* \psi_2^* \psi_1 dx$$

$$\text{or, } \lambda_1 \int_{-\infty}^{\infty} \psi_2^* \psi_1 dx = \lambda_2^* \int_{-\infty}^{\infty} \psi_2^* \psi_1 dx$$

$$\text{or, } (\lambda_1 - \lambda_2^*) \int_{-\infty}^{\infty} \psi_2^* \psi_1 dx = 0$$

$$\lambda_1 \neq \lambda_2^* \quad \text{So, } \int_{-\infty}^{\infty} \psi_2^* \psi_1 dx = 0$$

i.e. ψ_1 and ψ_2 are orthogonal

Commutating operators:

Two operators $\hat{A}$ and $\hat{B}$ are said to be commuting operator if

$$\hat{\alpha} \hat{\beta} = \hat{\beta} \hat{\alpha}$$

$$\text{or, } \hat{\alpha} \hat{\beta} - \hat{\beta} \hat{\alpha} = 0$$

$$\text{or, } [\hat{\alpha}, \hat{\beta}] = 0$$

$$\Rightarrow [\hat{\alpha}, \hat{\beta}] \psi = 0$$

$$\psi \neq 0, [\hat{\alpha}, \hat{\beta}] = 0$$

★ The physical meaning of this is that, these values can be measured simultaneously.

Similarly,

$$\text{if } \hat{\alpha} \hat{\beta} \neq \hat{\beta} \hat{\alpha}$$

$$\text{i.e. } [\hat{\alpha}, \hat{\beta}] \neq 0$$

Then, these operators are non-commutative

- Q (1) Find the value of
- (i) $[\hat{x}, \hat{p}_x]$
 - (ii) $[\hat{y}, \hat{p}_x]$
 - (iii) $[\hat{p}_x, \hat{p}_x]$
 - (iv) $[\hat{p}_x, \hat{p}_y]$

(i) $[\hat{x}, \hat{p}_x] \psi$

$$= (\hat{x} \hat{p}_x - \hat{p}_x \hat{x}) \psi$$

$$= \hat{x} \hat{p}_x \psi - \hat{p}_x \hat{x} \psi$$

$$= x \left(-i\hbar \frac{\partial \psi}{\partial x} \right) - \left\{ -i\hbar \frac{\partial}{\partial x} (x \psi) \right\}$$

$$= -i\hbar x \frac{\partial \psi}{\partial x} + i\hbar \psi \frac{\partial x}{\partial x} + i\hbar x \frac{\partial \psi}{\partial x}$$

$$\therefore \hat{H} = \frac{\hat{p}_x^2}{2m} + V(x) = \frac{\left(-i\hbar \frac{\partial}{\partial x}\right)^2}{2m} + V(x)$$

$$= -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

Proof :

$$\hat{H}_x \psi(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x) \psi(x).$$

Multiplying with $\hat{\pi}$,

$$\hat{\pi} \hat{H}_x \psi(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial (-x)^2} \psi(-x) + V(-x) \psi(-x)$$

$$= \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(-x) \right\} \psi(-x).$$

$$= \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \pi \psi(x); V(x) = V(-x)$$

$$\hat{\pi} \hat{H}_x \psi(x) = \hat{H}_x \hat{\pi} \psi(x)$$

$$(\hat{\pi} \hat{H}_x - \hat{H}_x \hat{\pi}) \psi(x) = 0$$

$$\Rightarrow [\hat{\pi}, \hat{H}_x] \psi(x) = 0.$$

$$\Rightarrow [\hat{\pi}, \hat{H}_x] = 0. \quad [\because \psi(x) \neq 0]$$

... Proved, ..

$$= i\hbar \psi$$

$$\text{or, } [\hat{x}, \hat{p}_x] \psi = i\hbar \psi$$

$$[\hat{x}, \hat{p}_x] = i\hbar$$

$$\textcircled{ii} [\hat{y}, \hat{p}_x] \psi$$

$$= (\hat{y} \hat{p}_x - \hat{p}_x \hat{y}) \psi$$

$$= \hat{y} \hat{p}_x \psi - \hat{p}_x \hat{y} \psi$$

$$= y \left(-i\hbar \frac{d\psi}{dx} \right) - \int -i\hbar \frac{d}{dx} (y \psi)$$

$$= -i\hbar y \frac{d\psi}{dx} + i\hbar y \frac{d\psi}{dx}$$

$$= 0$$

$$\text{or, } [\hat{y}, \hat{p}_x] = 0$$

$$\textcircled{iii} [\hat{p}_x, \hat{p}_x] \psi$$

$$= (\hat{p}_x \hat{p}_x - \hat{p}_x \hat{p}_x) \psi$$

$$= 0$$

$$\therefore [\hat{p}_x, \hat{p}_x] = 0$$

$$\begin{aligned}
 \textcircled{\text{iv}} \quad [\hat{P}_x, \hat{P}_y] \psi &= (\hat{P}_x \hat{P}_y - \hat{P}_y \hat{P}_x) \psi \\
 &= \hat{P}_x \hat{P}_y \psi - \hat{P}_y \hat{P}_x \psi \\
 &= \hat{P}_x \left(-i\hbar \frac{d\psi}{dy} \right) - \hat{P}_y \left(-i\hbar \frac{d\psi}{dx} \right) \\
 &= (-i\hbar)^2 \frac{d^2\psi}{dx dy} - (-i\hbar)^2 \frac{d^2\psi}{dy dx} \\
 &= -\hbar^2 \frac{d^2\psi}{dx dy} + \hbar^2 \frac{d^2\psi}{dy dx}
 \end{aligned}$$

$$\begin{aligned}
 \textcircled{\text{v}} \quad [x^2, p_x] \psi &= ? \\
 &= (x^2 \hat{P}_x - \hat{P}_x x^2) \psi \\
 &= x^2 \hat{P}_x \psi - \hat{P}_x x^2 \psi \\
 &= x^2 \left(-i\hbar \frac{d\psi}{dx} \right) + \left(i\hbar \frac{d(x^2 \psi)}{dx} \right) \\
 &= -i\hbar x^2 \cancel{\frac{d\psi}{dx}} + x^2 i\hbar \cancel{\frac{d\psi}{dx}} + i\hbar \psi \times 2x \\
 &= 2i\hbar x \cdot \psi \\
 [x^2, p_x] \psi &= 2i\hbar x \psi \\
 \therefore [x^2, p_x] &= 2i\hbar x
 \end{aligned}$$

$$\text{vi)} \quad [x^n, p_x] \psi = ?$$

$$= (x^n \hat{p}_x - \hat{p}_x x^n) \psi$$

$$= x^n \hat{p}_x \psi - \hat{p}_x x^n \psi$$

$$= x^n \left(-i\hbar \frac{d}{dx} \right) \psi + i\hbar \left(\frac{d}{dx} x^n \psi \right)$$

$$= -i\hbar x^n \frac{d\psi}{dx} + x^n i\hbar \frac{d\psi}{dx} + i\hbar \psi n x^{n-1}$$

$$= i\hbar n x^{n-1} \psi$$

$$\therefore [x^n, p_x] = n x^{n-1} i\hbar$$

$$\text{(vii)} \quad [x, p_x^n] \psi = ?$$

$$= (x p_x^n - p_x^n x) \psi$$

$$= x p_x^n \psi - p_x^n x \psi$$

$$= x \left(-i\hbar \frac{d}{dx} \right)^n \psi - \left(-i\hbar \frac{d}{dx} \right)^n x \psi$$

$$= (-i\hbar)^n x \frac{d^n \psi}{dx^n} - (-i\hbar)^n \left\{ \frac{d^n}{dx^n} (x \psi) \right\}$$

$$= (-i\hbar)^n x \frac{d^n \psi}{dx^n} - (-i\hbar)^n \left\{ n x \frac{d^{n-1} \psi}{dx^{n-1}} + \frac{d^{n-1} \psi}{dx^{n-1}} \right\}$$

$$\begin{aligned}
 &= (-i\hbar)^n x \frac{d^n \psi}{dx^n} - (-i\hbar)^n \left[n c_0 \frac{d^{n-1} \psi}{dx^{n-1}} + n c_1 \frac{d^{n-1} x}{dx^{n-1}} \frac{d\psi}{dx} \right. \\
 &\quad \left. + n c_2 \frac{d^{n-2} x}{dx^{n-2}} \frac{d^2 \psi}{dx^2} + \dots + n c_{n-1} \frac{dx}{dx} \frac{d^{n-1} \psi}{dx^{n-1}} + n c_n \frac{d^n \psi}{dx^n} \right] \\
 &= (-i\hbar)^n x \frac{d^n \psi}{dx^n} - (-i\hbar)^n n \frac{d^{n-1} \psi}{dx^{n-1}} - (-i\hbar)^n x \frac{d^n \psi}{dx^n}
 \end{aligned}$$

$$\begin{aligned}
 &= -(-i\hbar)^n n \frac{d^{n-1} \psi}{dx^{n-1}} \\
 &= -n (-i\hbar) (-i\hbar)^{n-1} \frac{d^{n-1} \psi}{dx^{n-1}} \\
 &= n i \hbar \frac{d^{n-1} \psi}{dx^{n-1}}
 \end{aligned}$$

$$\Rightarrow [x, P_x^n] = n i \hbar P_x^{n-1}$$

Angular Momentum Operator:

$$\vec{L} = \vec{r} \times \vec{p} = (x\hat{i} + y\hat{j} + z\hat{k}) (P_x\hat{i} + P_y\hat{j} + P_z\hat{k})$$

$$= \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ P_x & P_y & P_z \end{vmatrix}$$

$$= \hat{i} (yP_z - zP_y) + \hat{j} (zP_x - xP_z) + \hat{k} (xP_y - yP_x)$$

$$\vec{L} = L_x \hat{i} + L_y \hat{j} + L_z \hat{k}$$

where $L_x = yP_z - zP_y$

$$L_y = zP_x - xP_z$$

$$L_z = xP_y - yP_x$$

- 1) $[L_x, L_x] = ?$
- 2) $[L_x, L_y] = ?$
- 3) $[L_x, L_z] = ?$
- 4) $[L_x, P_x] = ?$

1) soln:

$$[L_x, L_x]\psi = (xL_x - L_x x)\psi$$

$$= \{x(yP_z - zP_y) - (yP_z - zP_y)x\}\psi$$

$$= (xyP_z - xzP_y - yP_zx - zP_yx)\psi$$

$$= -i\hbar \left(xy \frac{d\psi}{dz} - xz \frac{d\psi}{dy} - y \frac{d}{dz}(x\psi) + z \frac{d}{dy}(x\psi) \right)$$

$$= -i\hbar \left(xy \frac{d\psi}{dz} - xz \frac{d\psi}{dy} - yx \frac{d\psi}{dz} - y\psi \frac{dx}{dz} + z\psi \frac{dx}{dy} + zx \frac{d\psi}{dy} - z\psi \frac{dx}{dy} \right)$$

$$= 0$$

Properties

$$(i) [\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$$

$$\text{L.H.S} = [\hat{A}, \hat{B}] \psi = (\hat{A}\hat{B} - \hat{B}\hat{A}) \psi$$

$$= -(\hat{B}\hat{A} - \hat{A}\hat{B}) \psi$$

$$= -[\hat{B}, \hat{A}] \psi$$

$$\Rightarrow [\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$$

$$(ii) [\hat{A} \pm \hat{B}, \hat{C}] = [\hat{A}, \hat{C}] \pm [\hat{B}, \hat{C}]$$

$$\text{L.H.S} = [\hat{A} \pm \hat{B}, \hat{C}] \psi = \{(\hat{A} \pm \hat{B})\hat{C} - \hat{C}(\hat{A} \pm \hat{B})\} \psi$$

$$= (\hat{A}\hat{C} \pm \hat{B}\hat{C} - \hat{C}\hat{A} \mp \hat{C}\hat{B}) \psi$$

$$= \{(\hat{A}\hat{C} - \hat{C}\hat{A}) \pm (\hat{B}\hat{C} - \hat{C}\hat{B})\} \psi$$

$$= \{[\hat{A}, \hat{C}] \pm [\hat{B}, \hat{C}]\} \psi$$

$$\Rightarrow [\hat{A} \pm \hat{B}, \hat{C}] = [\hat{A}, \hat{C}] \pm [\hat{B}, \hat{C}]$$

$$(iii) [\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$$

$$\text{R.H.S} = \{[\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]\} \psi$$

$$= (\hat{A}\hat{C}\hat{B} - \hat{C}\hat{A}\hat{B} + \hat{A}\hat{B}\hat{C} - \hat{A}\hat{C}\hat{B}) \psi$$

$$= (\hat{A} \hat{B} \hat{C} - \hat{C} \hat{A} \hat{B}) \psi$$

$$= [\hat{A} \hat{B}, \hat{C}] \psi$$

$$[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}] \quad (1)$$

$$\Rightarrow [\hat{A} \hat{B}, \hat{C}] = [\hat{A}, \hat{C}] \hat{B} + \hat{A} [\hat{B}, \hat{C}]$$

$$4. [\hat{A}, \hat{B} \hat{C}] = [\hat{A}, \hat{B}] \hat{C} + \hat{B} [\hat{A}, \hat{C}]$$

$$5. [\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = 0$$

$$6. [\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$$

$$\text{Parity Operator : } \hat{\pi} : \hat{\pi} + [\hat{\pi}, \hat{A}] = [\hat{\pi}, \hat{A} \pm \hat{A}] \quad (11)$$

An operator represented by $\hat{\pi}$ is called parity operator and it operates as follows:

$$\hat{\pi} \psi(x, y, z) = \psi(-x, -y, -z) \quad \text{even parity}$$

$$= -\psi(-x, -y, -z) \quad \text{odd parity}$$

$$\psi(x, y, z) = \sin x$$

$$\pi \cos x = \cos(-x)$$

$$\hat{\pi}(\sin x) = \sin(-x)$$

$$= -\sin x$$

Properties of parity operator:

(1) It is linear operator.

$$\hat{\pi}(\psi_1(x) + \psi_2(x)) = \hat{\pi}\psi_1(x) + \hat{\pi}\psi_2(x)$$

$$\hat{\pi} \psi(x) = (\hat{\pi} \psi)(x)$$

(2) Parity operator is Hermitian operator.

$$\text{i.e. } \int_{-\infty}^{\infty} \psi_1^*(x) \hat{\pi} \psi_2(x) dx = \int_{-\infty}^{\infty} (\hat{\pi} \psi_1(x))^* \psi_2(x) dx$$

Proof:

$$\text{L.H.S} = \int_{-\infty}^{\infty} \psi_1^*(x) \hat{\pi} \psi_2(x) dx = \int_{-\infty}^{\infty} \psi_1^*(x) \psi_2(-x) dx$$

$$\text{let } -x = x'$$

$$\Rightarrow -dx = dx'$$

$$\text{or, } dx = -dx'$$

when,

$$-x = x' \rightarrow +\infty \text{ (lower limit)}$$

$$x' \rightarrow x$$

when

$$x' \rightarrow -x = -(-\infty) \rightarrow \infty$$

(lower limit)

$$x' \rightarrow -x = -(\infty) = -\infty$$

(upper limit)

then,

$$\begin{aligned} &= \int_{+\infty}^{-\infty} \psi_1^*(-x') \psi_2(x') dx' \\ &= \int_{-\infty}^{+\infty} \psi_1^*(-x') \psi_2(x') dx' \end{aligned}$$

Proved

$$= \int_{-\infty}^{\infty} \psi_1^*(-x) \psi_2(x) dx ; x' = x \text{ is a dummy variable}$$

$$= \int_{-\infty}^{\infty} (\pi \psi_1(x))^* \psi_2(x) dx.$$

$$= R.H.S.$$

(3) Parity operator commutator with Hamiltonian operator.

$$[\pi, \hat{H}] = 0.$$

$$H = T + V$$

$$= \frac{p^2}{2m} + V$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}$$

$$\hat{H} = \frac{(-i\hbar \nabla)^2}{2m} + V$$

$$p = -i\hbar \nabla$$

$$p_x = -i\hbar \frac{\partial}{\partial x}$$

$$p_y = -i\hbar \frac{\partial}{\partial y}$$

$$p_z = -i\hbar \frac{\partial}{\partial z}$$